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A STUDY OF MAGNETIC INTERACTIONS IN HEXAGONAL IRON ALLOYS

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Résumé.- Des alliages de structure hexagonale à base de fer (phase ϵ) contenant de 15 à 30 at. % de ruthénium ou d'osmium ont été étudiés par effet Mössbauer du ^{57}Fe . Il apparaît un ordre antiferromagnétique dans Fe-Ru et il en est probablement de même dans Fe-Os. Les valeurs mesurées du champ hyperfin à saturation et de la température de Néel ont été 15 kG et 210 K, 13 kG et 60 K, 3,3 kG et 30 K pour des alliages contenant 15 et 30 at. % de Ru, ou 15 at. % de Os respectivement. Dans tous les cas, la direction d'aimantation semble être orientée à environ 50° du gradient de champ électrique. L'alliage $\text{Fe}_{0,7}\text{Os}_{0,3}$ ne possède pas de température d'ordre. Les résultats obtenus sont extrapolés et discutés à partir des théories habituelles traitant de la mise en ordre magnétique dans le fer pur hcp qui est seulement obtenu par application de pressions hydrostatiques élevées (>130 kbar).

Abstract.- Hexagonal (ϵ -phase) alloys of iron with 15 and 30 atomic percent of ruthenium or osmium have been studied using the ^{57}Fe Mössbauer resonance. The existence of antiferromagnetic ordering in the Fe-Ru and probably in the Fe-Os alloys is indicated. The saturated hyperfine fields and Néel temperatures for the 15 and 30 at. % Ru and the 15 at. % Os alloys were 15 kG and 210 K, 13 kG and 60 K, 3.3 kG and 30 K, respectively. In each case the direction of magnetization seems to be oriented at about 50 degrees to the e.f.g. The alloy $\text{Fe}_{0,7}\text{Os}_{0,3}$ showed no evidence of ordering at any temperature. The results obtained have been extrapolated to those to be expected for pure hcp iron and will be discussed in relation to current theoretical treatment of magnetic ordering in the ϵ -phase of iron, normally realizable only by the application of large external pressures ($P > 130$ kbar).

1. Introduction.- Three phases of pure iron (α , γ and ϵ) have been observed under different physical conditions and although widely studied using various techniques many of the microscopic properties are still not fully understood. In particular the magnetic properties of such a transition metal are obviously of considerable interest. With reference to the phase diagram /1/ we see that under normal conditions at room temperature and atmospheric pressure, pure iron is stable in the bcc α -phase. This phase is ferromagnetic, apart from a small region above 1000 K, where the Curie transformation takes place before the α - γ (fcc) transformation. The high temperature/high pressure γ -phase was found to be paramagnetic. However, a form of γ -Fe which is stable at low temperatures can be produced by precipitation in copper. Gonser et al. /2/ and Johnson et al. /3/ found that this form ordered antiferromagnetically below ~ 70 K with a corresponding saturated hyperfine field ~ 24 kG.

Recently, much interest has been shown in the hcp ϵ -phase of iron, which is stable only at pressures in excess of ~ 130 kbars, particularly as regards its magnetic properties. This phase was originally shown to be paramagnetic at room temperature by Nicol et al. /4/ and Pipkorn et al. /5/.

Mössbauer experiments have now been carried

out on pure hcp Fe at low temperatures /1/ /6/ and rather surprisingly, showed little evidence of any magnetic ordering down to 2 K. The experimental accuracy /6/ allowed an upper limit of 5 kG for the nuclear hyperfine field at 2 K.

In order to gain information about the ϵ -phase of pure Fe whilst, at the same time, avoiding the high pressures involved for its stabilization, we may look at the properties of hexagonal phase alloys of iron in the high Fe concentration region. Early measurements by Ohno et al. /7/ on such alloys suggested an antiferromagnetic coupling and an extrapolation to pure iron yielded a Néel temperature of ~ 100 K and a saturated internal field of ~ 16 kG, in clear disagreement with the results of /6/ and /1/. Theoretical calculations carried out both by Fletcher and Addis /8/ and Madsen and Anderson (see Grimvall, /9/) failed to predict any magnetically ordered state, on the basis of simple Stoner criteria, either for pure hcp Fe or hcp alloys. This seemed to contradict the alloy observations /7/ while supporting the conclusions of the experiments on pure ϵ -Fe.

In order to try to resolve some of the controversy regarding the magnetic properties of ϵ -Fe, it was deemed that a detailed Mössbauer study of the more easily stabilized hexagonal Fe alloy systems

was required.

2. Sample choice and preparation.- Fujimori et al. /10/ studied the different alloy structures stabilized under different preparation conditions for Fe-Ru alloys and on the basis of their results alloys of 15 and 30 atomic percent of Ru (and Os) in Fe were chosen for our investigation of the ϵ -phase. Appropriate weights of the elements were thoroughly mixed and alloyed before annealing, under safe hydrogen, at 1400°C for a period of 9 hours and quenching into water. The ϵ -phase was confirmed by X-ray analysis.

3. Results.- ^{57}Fe Mössbauer absorption spectra were obtained for all four alloys at temperatures ranging from 5 - 300 K. The high temperature spectra were shown to be quadrupole doublets whilst at low temperatures there was considerable line broadening, particularly for the Ru alloys. (Williams and Pearson, /11/).

Various sources of low temperature broadening were examined, namely, 1) increased "thickness" effects due to an increase in the recoil-free fraction; 2) inhomogeneous increases in the Q.S. due to anisotropic lattice contraction; 3) relaxation effects and 4) the onset of magnetic ordering. We conclude, however, that the bulk of the spectral broadening observed is due to the onset of magnetic ordering. The broadened spectra were thus assumed to arise from the co-existing electric quadrupole and magnetic hyperfine interactions, both having roughly the same order of magnitude. The fitting method suggested by van Dongen Torman et al. /12/ was used and the resulting hyperfine field dependence on temperature for the $\text{Fe}_{0.85}\text{Ru}_{0.15}$ alloy is shown in figure 1.

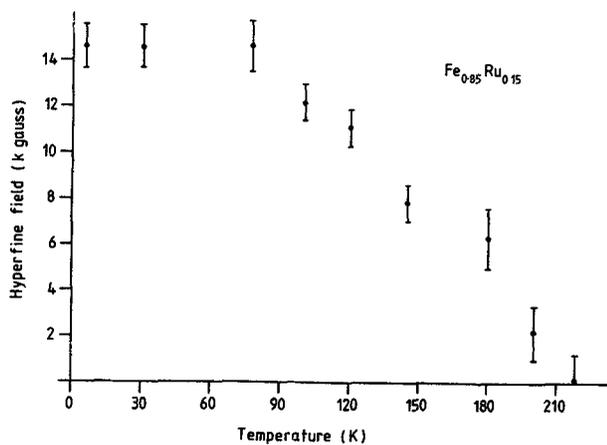


Fig. 1 : The measured hyperfine field-temperature dependence for the $\text{Fe}_{0.85}\text{Ru}_{0.15}$ alloy.

A comparison of the fitted spectra with Kundig's /13/ calculated plots suggested that the angle bet-

ween the magnetic field vector and the e.f.g. symmetry axis is $\sim 50^\circ$.

A complete analysis of the 15 and 30 at. % Ru and the 15 at. % Os alloys yielded saturated hyperfine fields and Néel temperatures of 15 kG and 210 K, 13 kG and 60 K and 3,3 kG and 30 K respectively.

4.- Discussion.- Our Fe-Ru results when extrapolated to those expected for pure ϵ -iron suggest an ordering temperature ~ 360 K with a saturation field ~ 17 kG.

The low temperature/high pressure Mössbauer studies of pure iron, showed no such evidence of magnetic ordering. These results seem, at first, to contradict the expected behaviour of pure ϵ -Fe from our study of the ϵ -phase alloys. However, we might consider our extrapolation to pure ϵ -Fe and the results for pure Fe at high pressure with reference to the plot of atomic moment versus atomic volume in figure 2 /9/.

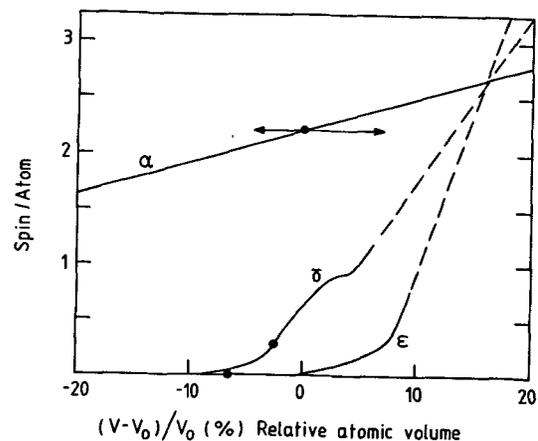


Fig. 2 : The ferromagnetic moment (spins per atom) for bcc, fcc and hcp iron as a function of atomic volume (from reference /9/). The arrows show the volume change under a pressure of 100 kbars and the thermal expansion up to 1800 K. Dashed lines indicate that the spin was not uniquely obtained.

We note, in particular, the form of the ϵ -phase curve which is close to zero ($< 0.1\mu_B$) for volumes below $\sim +5\%$, but shows a rapid increase in atomic moment with volume above this value. Thus, according to this theoretical curve, with an atomic volume corresponding to that of the high pressure ϵ -phase of pure Fe ($\sim -7\%$), we would expect the atomic moment to be close to zero, as was indeed observed. However, it is likely that an extrapolation to zero percent Ru (or indeed Os) would imply a pure Fe atomic volume well above that observed under the necessary conditions for its stabilization. This being the case, it is quite possible that our extrapolation would

fall above zero on the volume axis, and our values would apply to a "theoretical ϵ -phase" of Fe, physically unrealizable. Assuming proportionality between the Fe magnetic moment and the observed internal hyperfine field, our extrapolation yields a value of

$0.1\mu_B$ for the ϵ -Fe atomic moment, and from figure 2 this would imply that our extrapolation falls at a volume $\sim 5\%$ above that of ϵ -Fe under normal conditions.

We thus conclude that in the ϵ -phase Fe-Ru alloys there is Mössbauer evidence for magnetic ordering as suggested by earlier resistivity (Sarkissian and Coles /3/) and specific heat (Clauss /14/) data.

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